

Table 2. Comparison of PLS results of the secondary structure of proteins in H₂O and D₂O.

		α -Helix			β -Sheet		
PDBID	Protein Names	Observed (X-ray)	Predicted (H ₂ O)	Predicted (D ₂ O)	Observed (X-ray)	Predicted (H ₂ O)	Predicted (D ₂ O)
3CWL	alpha-1-antitrypsin	0.28	0.20	0.31	0.31	0.33	0.32
3M1K	carbonic anhydrase (human)	0.08	0.10	0.05	0.29	0.35	0.33
1YPH	Chymotrypsin (bovine)	0.00	0.05	0.05	0.35	0.35	0.36
1HRC	cytochrome (horse heart)	0.41	0.52	0.44	0.00	0.02	0.04
2QSP	Hemoglobin bovine	0.67	0.67	0.58	0.00	0.00	0.02
2LYZ	lysozyme (chicken egg)	0.32	0.41	0.43	0.06	0.07	0.04
1NZ2	Myoglobin (horse muscle)	0.74	0.57	0.70	0.00	0.03	0.00
3DLW	native-anti-chymotrypsin	0.29	0.29	0.17	0.36	0.24	0.32
1T1F	native form of anti-thrombin	0.26	0.27	0.21	0.27	0.34	0.38
2OAY	native form of c1 inhibitor	0.27	0.29	0.25	0.32	0.28	0.26
1yx9	Pepsin (pepsin gastric mucosa)	0.10	0.12	0.16	0.42	0.41	0.33
1RBX	ribonuclease A (bovine pancreas)	0.20	0.18	0.10	0.30	0.29	0.31
3DJV	ribonuclease S (bovine pancreas)	0.19	0.20	0.30	0.33	0.32	0.33
1ATH	split form of anti-thrombin	0.27	0.29	0.30	0.32	0.33	0.30
1LQ8	split form of c1 inhibitor	0.28	0.29	0.25	0.35	0.28	0.32
2tga	trypsinogen(bovine pancreas)	0.07	-0.01	0.13	0.32	0.35	0.34
	R ²		0.88	0.87		0.90	0.90
	RMSEP		0.066	0.069		0.044	0.045